

Huge quantum particle number fluctuations in a two-component Bose gas in a double-well potential

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Two component Bose gas in a double well potential with repulsive interactions may undergo a phase separation transition if the inter-species interactions outweigh the intra-species ones. We analyze the transition in the strong interaction limit within the two-mode approximation. Numbers of particles in each potential well are equal and constant. However, at the transition point, the ground state of the system reveals huge fluctuations of numbers of particles belonging to the different gas components. That is, probability for observation of any mixture of particles in each potential well becomes uniform.

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I. INTRODUCTION

Ultra-cold dilute gases of bosonic atoms constitute perfect systems for experimental and theoretical investigations of various phenomena of quantum many body problems [1]. From the viewpoint of quantum computing and interferometry an especially relevant subject is quantum fluctuations [2, 3].

Most experimental studies of fluctuations concentrated on systems of cold atoms in double well [4] and optical lattice potentials [5]. In the former system squeezed states were predicted and produced, with particle number fluctuations (i.e. uncertainties of populations of the potential wells) turning from poissonian to sub-poissonian [6–8]. The latter system reveals a superfluid to Mott insulator transition [9–11] with enhanced phase fluctuations but with decreasing particle number fluctuations.

In the present paper we focus on a system where the total particle number is fixed but occupation of certain single particle states reveals considerable quantum fluctuations. We are interested in a system where the mean field theory predicts symmetry breaking [12–14] and the symmetry broken solutions are degenerated and form a Hilbert subspace parameterized by a continuous parameter. If the occupation of single particle states varies a lot as we move in the degenerate subspace than huge particle number fluctuations can be expected in the exact quantum many body eigenstates. Degenerate subspace parameterized by a continuous parameter appears in spin-1 Bose gas with an anti-ferromagnetic interaction [15] or in scalar condensates with solitonic solutions [15–17]. Attractive single component Bose gas in a symmetric double well potential reveals also huge particle number fluctuations but it constitutes a slightly different example [18, 19]. There the degeneracy is small, i.e. the degenerate subspace is two dimensional, and the particle number fluctuations correspond to random localization of all particles in one of the potential wells in different experimental realizations. In all these examples the cor-

rect mean field theory reduces to the Gross-Pitaevskii equations [1]. In the present paper we consider a Bose gas system where the Gross-Pitaevskii equation is not a correct mean-field description, that is, a two-component Bose gas in a double-well potential in the strong interaction limit.

In Sec. II we present a theoretical model for a two-component Bose gas in a double-well potential. In Sec. III A we derive the effective Hamiltonian using second order perturbation theory valid in the strong interaction limit. In Sec. III B we analyze its mean field (classical) limit and identify phase transition region. It turns out that the mean-field solutions reveal continuous degeneracy at the transition point. We deduce the exact ground state of the system in Sec. III C and show that the particle number fluctuations are indeed huge at the critical point. In Sec. III D we estimate the range of parameters where the predicted fluctuations can be observed and in Sec. IV the results presented in the paper are summarized.

II. THE MODEL

The Hamiltonian of a two component Bose gas in a symmetric double well potential, in the tight binding approximation, takes the form of the Bose-Hubbard model

$$\begin{aligned} \hat{H} = & -\frac{J}{2} \left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 + \hat{b}_1^\dagger \hat{b}_2 + \hat{b}_2^\dagger \hat{b}_1 \right) \\ & + \frac{U}{2} \left(\hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2 + \hat{b}_1^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{b}_1 + \hat{b}_2^\dagger \hat{b}_2^\dagger \hat{b}_2 \hat{b}_2 \right) \\ & + U_{ab} \left(\hat{a}_1^\dagger \hat{a}_1 \hat{b}_1^\dagger \hat{b}_1 + \hat{a}_2^\dagger \hat{a}_2 \hat{b}_2^\dagger \hat{b}_2 \right), \end{aligned} \quad (1)$$

where we have assumed that intra-species interactions are the same in both gas components and they are characterized by a coupling constant U . The parameter U_{ab} is a coupling constant that describes inter-species interactions while J stands for the tunneling rate between the two potential wells. We assume also that numbers of particles of each component are equal to $2N$. Such a choice

of the system parameters allows us to perform fully analytical calculations. Analysis of a general case is beyond the scope of the present paper. The Hamiltonian (1) can be transformed to

$$\hat{H} = -\frac{J}{2}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 + \hat{b}_1^\dagger \hat{b}_2 + \hat{b}_2^\dagger \hat{b}_1) + \frac{U_s}{8}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2 + \hat{b}_1^\dagger \hat{b}_1 - \hat{b}_2^\dagger \hat{b}_2)^2 + \frac{U_d}{8}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2 - \hat{b}_1^\dagger \hat{b}_1 + \hat{b}_2^\dagger \hat{b}_2)^2, \quad (2)$$

where $U_s = U + U_{ab}$, $U_d = U - U_{ab}$ and constant terms have been omitted. In the following we consider U_s as the unit of energy.

III. PERTURBATION APPROACH

A. The second order effective Hamiltonian

We are interested in the strong interaction limit. Therefore, the tunneling part of the Hamiltonian will be considered as a small perturbation. For $J = 0$ the system Hamiltonian has exact eigenstates

$$|N + n_a, N - n_a\rangle |N + n_b, N - n_b\rangle, \quad (3)$$

where $N + n_a$, $N - n_a$ refer to numbers of particles of the component a in the first and the second potential well, respectively, and similarly for the component b . The energies of such states (remember that U_s is the unit of energy) are

$$E = \frac{1}{2}(n_a + n_b)^2 + \frac{U_d}{2}(n_a - n_b)^2. \quad (4)$$

Switching to variables $n_s = n_a + n_b$, $n_d = n_a - n_b$ we obtain eigenenergies in a very simple form

$$E = \frac{1}{2}n_s^2 + \frac{U_d}{2}n_d^2. \quad (5)$$

If we assume that the parameters satisfy the condition

$$1 \gg |U_d|N^2, \quad (6)$$

then manifolds with different values of $|n_s|$ are separated on the energy scale (see Fig. 1). The lowest energy manifold is related to $n_s = 0$ and states within each manifold are labelled by different values of n_d .

Matrix elements of the tunneling part of the Hamiltonian are zero between states of the same manifold. However, this part of the Hamiltonian introduces couplings between different manifolds. In an effective Hamiltonian that describes the lowest manifold of the system the effect of the coupling can be included via the second order perturbation theory. A compact form of the effective Hamiltonian may be obtained if we introduce spin operators

$$\hat{S}_{jx} = \frac{1}{2}(\hat{a}_j^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_j),$$

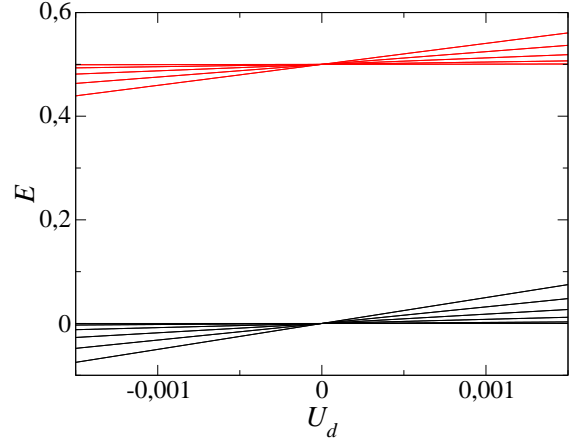


FIG. 1: (Color online) Energy levels (5) versus U_d for a number of particles of each component equal $2N = 100$. Black lines: the lowest energy manifold, i.e. $n_s = 0$, red lines: the manifold corresponding to $|n_s| = 1$.

$$\begin{aligned} \hat{S}_{jy} &= -\frac{i}{2}(\hat{a}_j^\dagger \hat{b}_j - \hat{b}_j^\dagger \hat{a}_j), \\ \hat{S}_{jz} &= \frac{1}{2}(\hat{a}_j^\dagger \hat{a}_j - \hat{b}_j^\dagger \hat{b}_j). \end{aligned} \quad (7)$$

States belonging to the lowest manifold ($n_s = 0$) can be written in the Fock basis (3) as

$$|\psi\rangle = \sum_{n=-N}^N \psi(n) |N + n, N - n\rangle |N - n, N + n\rangle. \quad (8)$$

The Fock states $|N + n, N - n\rangle |N - n, N + n\rangle$ are the eigenstates of the $\hat{\mathbf{S}}_j^2$, \hat{S}_{1z} and \hat{S}_{2z} operators with the corresponding eigenvalues $N(N+1)$, n and $-n$, respectively, so the $n_s = 0$ manifold can be specified by:

$$\hat{S}_{1z} + \hat{S}_{2z} = 0, \quad \hat{\mathbf{S}}_j^2 = N(N+1). \quad (9)$$

In the second order in J the effective Hamiltonian that describes the lowest manifold reads [20–24]

$$\hat{H}_2 = -2J^2 \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 + U_d(\hat{S}_{1z}^2 + \hat{S}_{2z}^2). \quad (10)$$

The above Hamiltonian together with the condition (9) defines our problem where each potential well is associated with an angular momentum operator and there is interaction between such subsystems due to tunneling of atoms. Note that eigenstates of the Hamiltonian (10) depend on two parameters only, i.e. $U_d/(2J^2)$ and N .

B. Classical limit

Let us analyze the Hamiltonian (10) [in the manifold defined in (9)] in the classical limit by substituting the spin operators by classical angular momentum components. The condition (9) implies that $S_{1z} = -S_{2z}$. We

are interested in the ground state of the system. The value of the tunneling part of the Hamiltonian

$$-2J^2 \mathbf{S}_1 \cdot \mathbf{S}_2 = -2J^2(S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}), \quad (11)$$

is minimal for $S_{1x} = S_{2x}$, $S_{1y} = S_{2y}$. For $U_d/(2J^2) + 1 < 0$ the ground state corresponds to $|S_{jz}| = N$ which can be related to $n_d = \pm 2N$ (i.e. phase separation occurs where different gas components occupy different potential wells). For $U_d/(2J^2) + 1 > 0$ the z -components of the angular momenta disappear in the ground state ($S_{jz} = 0$) which corresponds to $n_d = 0$ (i.e. equal mixture of both components in each potential well). When $U_d/(2J^2) + 1 = 0$ we deal with the transition point where $|S_{jz}|$ can be arbitrary provided $S_{1z} + S_{2z} = 0$. Then all values of n_d are equally probable (any mixture of both components in each potential well is equally likely). The transition between the phase separation and miscible regimes is discontinuous.

C. Quantum ground state

The analysis of the classical limit suggests that huge particle number fluctuations can be expected in the quantum ground state of the system at the transition point. Let us switch now to quantum analysis of the Hamiltonian (10). For $U_d = -2J^2$ the Hamiltonian reads

$$\hat{H}_2 = J^2[(\hat{S}_{1x} - \hat{S}_{2x})^2 + (\hat{S}_{1y} - \hat{S}_{2y})^2 - \hat{\mathbf{S}}_1^2 - \hat{\mathbf{S}}_2^2]. \quad (12)$$

Applying the unitary (rotation) transformation

$$\hat{S}_{1x} \rightarrow -\hat{S}_{1x} \quad \hat{S}_{1y} \rightarrow -\hat{S}_{1y} \quad \hat{S}_{1z} \rightarrow \hat{S}_{1z}, \quad (13)$$

which commutes with \hat{S}_{jz} and thus leaves the manifold $\hat{S}_{1z} + \hat{S}_{2z} = 0$ invariant, and defining the total spin operator, $\hat{\mathbf{S}} = \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2$, we can rewrite the Hamiltonian (12) in the following form

$$\hat{H}_2 = J^2(\hat{\mathbf{S}}^2 - \hat{\mathbf{S}}_1^2 - \hat{\mathbf{S}}_2^2). \quad (14)$$

States $|j, 0\rangle$ with an integer j , where $j(j+1)$ is an eigenvalue of the $\hat{\mathbf{S}}^2$ operator and 0 is an eigenvalue of the $\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z}$ operator, are therefore eigenstates of our problem. The energy spectrum reads

$$E_j = J^2(j(j+1) - 2N(N+1)), \quad (15)$$

with $0 \leq j \leq 2N$ and the ground state solution corresponds to $j = 0$. In the basis (3) it takes the form of

$$|\psi_0\rangle = \frac{1}{\sqrt{2N+1}} \sum_{n=-N}^N |N+n, N-n\rangle |N-n, N+n\rangle. \quad (16)$$

Huge particle number fluctuations become apparent in Eq. (16) where the ground state turns out to be a uniform superposition of all Fock states belonging to the lowest

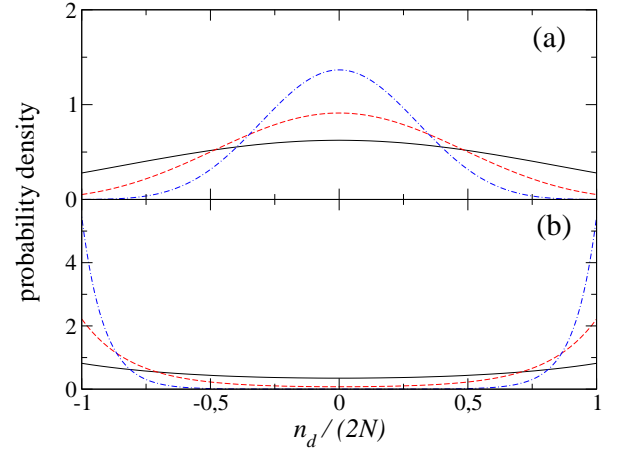


FIG. 2: (Color online) Ground state probability density $\rho(n_d) = |\psi_0(n_d)|^2$ for $\frac{U_d}{2J^2} + 1 = 10^{-3}$ (a) and $\frac{U_d}{2J^2} + 1 = -10^{-3}$ (b). Solid black lines are related to the number of particles in each gas component $2N = 50$, dashed red lines to $2N = 100$ and dotted-dashed blue lines to $2N = 200$.

energy manifold ($n_s = 0$). That is, all values of n_d are equally probable.

It is interesting to note that we can construct the exact quantum ground state using the superposition of symmetry broken solutions obtained in the classical limit. At the transition point the classical analysis tells us that in the ground state the potential wells are associated with classical angular momenta where orientation of one is given by $(\theta_1, \phi_1) = (\theta, \phi)$ and the other one by $(\theta_2, \phi_2) = (\pi - \theta, \phi)$ and spherical angles θ and ϕ can be arbitrary. The best quantum approximation of a classical angular momentum is a coherent state [25, 26]

$$|\theta_j, \phi_j\rangle = \frac{1}{\sqrt{(2N)!}} \left(\cos \frac{\theta_j}{2} e^{i\phi_j/2} \hat{a}_j^\dagger + \sin \frac{\theta_j}{2} e^{-i\phi_j/2} \hat{b}_j^\dagger \right)^{2N} |0\rangle. \quad (17)$$

If we postulate that the quantum ground state of our system can be approximated by a single tensor product state $|\theta, \phi\rangle |\pi - \theta, \phi\rangle$ the rotational symmetry of the Hamiltonian (10) will be broken. A rotationally invariant state can be restored if we prepare a uniform superposition of the tensor product states, i.e. by integrating over all solid angles

$$|\psi_0\rangle = \frac{\sqrt{2N+1}}{2} \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^\pi \sin \theta d\theta |\theta, \phi\rangle |\pi - \theta, \phi\rangle, \quad (18)$$

where $\langle \psi_0 | \psi_0 \rangle = 1$. Substituting Eq. (17) into Eq. (18), integrating over ϕ and employing the identity

$$\int_{-1}^1 d(\cos \theta) \left(\frac{1 + \cos \theta}{2} \right)^{N+n} \left(\frac{1 - \cos \theta}{2} \right)^{N-n} = \frac{2}{2N+1} \left[\binom{2N}{N+n} \right]^{-1}, \quad (19)$$

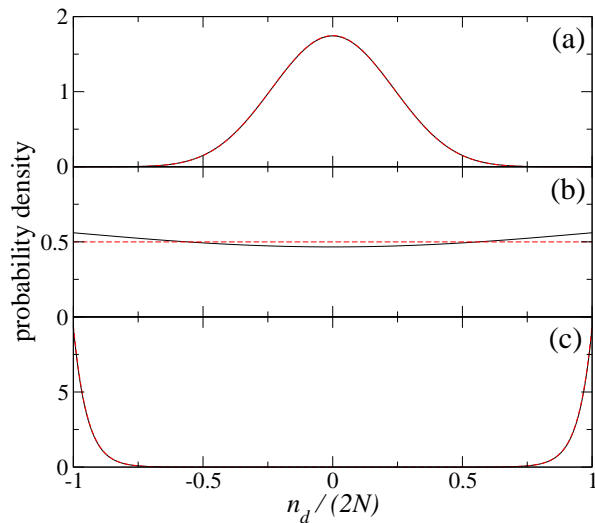


FIG. 3: (Color online) Ground state probability densities for a number of particles in each component $2N = 1000$, $J = 5 \times 10^{-7}$ and $\frac{U_d}{2J^2} = -0.9999$ (a), $\frac{U_d}{2J^2} = -1$ (b) and $\frac{U_d}{2J^2} = -1.0001$ (c). Solid black lines correspond to $\rho(n_d) = \sum_{n_s} |\psi_0(n_s, n_d)|^2$ where $\psi_0(n_s, n_d)$ is obtained by diagonalization of (2) while dashed red lines are related to $\rho(n_d) = |\psi_0(n_d)|^2$ with $\psi_0(n_d)$ obtained by diagonalization of the effective Hamiltonian (10). In panels (a) and (c) the black and red lines are hardly distinguishable.

that follows from the completeness relation of the coherent states we restore the quantum ground state (16).

We see that at the transition point the classical analysis allows us to construct the exact ground state of the system. However, in the close vicinity of the transition point this analysis is not able to provide a good estimate for the ground state of the system. This is because the classical approach predicts discontinuous transition between the phase separation and miscible regimes but the transition is actually continuous. Starting with the classical ground states and using the coherent states we can construct quantum ground states that depend on N and on the sign of the parameter $U_d/(2J^2) + 1$ but not on its absolute value. However, the exact diagonalization indicates that there is a range of $U_d/(2J^2) + 1$ where the ground state changes continuously from the miscible to phase separation character. As one can expect this range shrinks with N because differences between the classical and quantum angular momentum diminish in the large N limit. This is illustrated in Fig. 2 where we plot $\rho(n_d) = |\psi_0(n_d)|^2$ for $U_d/(2J^2) + 1 = 10^{-3}$ and -10^{-3} , i.e. close to the transition point, for different values of N obtained in numerical diagonalization of the effective Hamiltonian (10).

D. Validity of the perturbation approach

Our predictions are based on the effective Hamiltonian (10) which is second order in J , and they are correct pro-

vided higher order terms can be neglected. The fourth order terms are smaller than $J^4(2N)^4$ or $J^2|U_d|(2N)^4$. At the transition point $|U_d| = 2J^2$, so if $J^4(2N)^4$ is much smaller than the energy gap between the ground and first excited states of the Hamiltonian (14), i.e. $E_1 - E_0 = 2J^2$, then the higher order terms can be neglected and the system is properly described by the second order Hamiltonian (14). Hence,

$$J^2(2N)^4 \ll 1, \quad (20)$$

is a sufficient condition for the validity of the ground state (16) that describes the huge particle number fluctuations in the system.

We have tested our predictions comparing them with exact numerical calculations. Figure 3 shows probability densities $\rho(n_d)$ corresponding to ground states of the system obtained by diagonalization of the full Hamiltonian (2) and the effective Hamiltonian (10) for $2N = 1000$ and $J = 5 \times 10^{-7}$. Different panels are related to different values of U_d in the vicinity of the transition point. That is, $\frac{U_d}{2J^2} + 1 = 10^{-4}$ corresponds to the miscible regime, $\frac{U_d}{2J^2} + 1 = 0$ to the transition point and $\frac{U_d}{2J^2} + 1 = -10^{-4}$ to the phase separation side of the transition point. We can see that on both sides of the transition point the density $\rho(n_d)$ is peaked around the classical solutions, while at the transition point it is uniformly distributed. Figure 3 indicates perfect agreement between the perturbation calculations and the exact results even though $J^2(2N)^4 = 0.25$ and thus the condition (20) is barely fulfilled.

IV. CONCLUSION

In summary, we have analyzed a strongly interacting two-component Bose gas in a double well potential for parameters close to the transition point where the phase separation occurs. The second order effective Hamiltonian allows us to describe the system in the vicinity of the transition point when higher order corrections are negligible. We have shown that, at the transition point, the ground state of the system becomes a uniform superposition of Fock states. That is, the system reveals huge quantum fluctuations of populations of the potential wells.

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